

Analytical and Bioanalytical Chemistry

Electronic Supplementary Material

Development and validation of a rapid multiplex ELISA for pyrrolizidine alkaloids and their *N*-oxides in honey and feed

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Table S1. The PA compounds and the mass spectrometric settings used

Number	Pyrrolizidine alkaloid	Abbreviation	Precursor ion (m/z)	Cone voltage (V)	Product ion 1 (m/z)	Collision energy 1 (eV)	Product ion 2 (m/z)	Collision energy 2 (eV)	Indicative RT (min)	Main PA Type	Reference standard for quantification
1	acetylchimidine	AcEch	440.2	30	120	25	220	20	11.15	lycopsamine	echimidine
2	acetylchimidine-N-oxide	AcEch-ox	456.2	30	254	30	338	25	8.20	lycopsamine	echimidine-N-oxide
3	acetylchinatine	AcEna	342.2	30	120	30	138	20	8.15	lycopsamine	lycopsamine
4	acetylchinatine-N-oxide	AcEna-ox	358.2	30	94	40	172	30	5.95	lycopsamine	lycopsamine-N-oxide
5	acetylerucifoline	AcEr	392.2	40	94	40	118	30	9.90	senecionine	erucifoline
6	acetylerucifoline-N-oxide	AcEr-ox	408.2	40	94	40	120	30	7.00	senecionine	erucifoline-N-oxide
7	acetylheliosupine	AcHsu	440.2	30	120	25	220	20	10.95	lycopsamine	echimidine
8	acetylheliosupine-N-oxide	AcHsu-ox	456.2	30	254	30	338	25	7.95	lycopsamine	echimidine-N-oxide
9	acetyllycopsamine	AcLyc	342.2	30	120	30	180	20	8.55	lycopsamine	lycopsamine
10	acetyllycopsamine-N-oxide	AcLyc-ox	358.2	30	137	30	214	30	6.20	lycopsamine	lycopsamine-N-oxide
11	acetylinderine	AcRin	342.2	30	120	30	138	20	8.35	lycopsamine	lycopsamine
12	acetylinderine-N-oxide	AcRin-ox	358.2	30	94	40	172	30	6.05	lycopsamine	lycopsamine-N-oxide
13	acetylseneciphylline	AcSp	376.2	40	120	30	138	30	11.52	senecionine	seneciphylline
14	acetylseneciphylline-N-oxide	AcSp-ox	392.2	40	94	40	118	30	8.62	senecionine	seneciphylline-N-oxide
15	dehydrojaconine	DHJn	386.2	40	94	40	120	30	7.65	senecionine	jacobine
16	desacetyldoronine	Dd	418.2	30	122	30	168	30	6.04	otonecine	florosene
17	doronine	Do	460.2	30	122	35	168	30	8.75	otonecine	florosene
18	echimidine	Ech	398.2	30	120	25	220	20	9.92	lycopsamine	echimidine
19	echimidine-N-oxide	Ech-ox	414.2	30	254	30	352	25	7.27	lycopsamine	echimidine-N-oxide
20	echinatine	Ena	300.2	30	138	30	156	30	6.95	lycopsamine	lycopsamine
21	echinatine-N-oxide	Ena-ox	316.2	30	111	40	172	30	4.96	lycopsamine	lycopsamine-N-oxide
22	echiumine	Eiu	382.2	30	94	30	120	30	10.35	lycopsamine	echimidine
23	echiumine-N-oxide	Eiu-ox	398.2	30	94	40	176	30	8.10	lycopsamine	echimidine-N-oxide
24	erucifoline	Er	350.2	40	94	40	138	30	7.25	senecionine	erucifoline
25	erucifoline-N-oxide	Er-ox	366.2	40	94	40	118	30	4.60	senecionine	erucifoline-N-oxide
26	europine	Eur	330.2	30	94	35	138	30	6.72	heliotrine	europine
27	europine-N-oxide	Eur-ox	346.2	30	172	30	256	25	4.81	heliotrine	europine-N-oxide
28	floridanine	Fd	442.2	30	122	30	168	30	6.60	otonecine	florosene
29	florosene	Fs	424.2	30	122	35	168	30	8.13	otonecine	florosene
30	heleusine-N-oxide	Heu-ox	314.2	30	120	30	156	25	6.65	heliotrine	heliotrine-N-oxide
31	heliosupine	Hsu	398.2	30	120	25	220	20	9.74	lycopsamine	echimidine
32	heliosupine-N-oxide	Hsu-ox	414.2	30	94	30	254	30	7.08	lycopsamine	echimidine-N-oxide
33	heliotrine	Hel	314.2	30	138	25	156	25	8.32	heliotrine	heliotrine
34	heliotrine-N-oxide	Hel-ox	330.2	30	111	35	172	25	5.95	heliotrine	heliotrine-N-oxide
35	indicine	Ind	300.2	30	94	35	156	30	6.35	lycopsamine	lycopsamine
36	indicine-N-oxide	Ind-ox	316.2	30	94	40	172	30	4.82	lycopsamine	lycopsamine-N-oxide
37	integerrimine	Ir	336.2	40	94	40	120	30	9.45	senecionine	integerrimine
38	integerrimine-N-oxide	Ir-ox	352.2	40	94	40	120	30	6.63	senecionine	integerrimine-N-oxide
39	intermediate	Int	300.2	30	94	35	156	30	6.35	lycopsamine	lycopsamine
40	intermediate-N-oxide	Int-ox	316.2	30	94	40	172	30	4.76	lycopsamine	lycopsamine-N-oxide
41	jacobine	Jb	352.2	40	120	30	155	30	7.57	senecionine	jacobine
42	jacobine-N-oxide	Jb-ox	368.2	40	120	30	296	25	5.30	senecionine	jacobine-N-oxide
43	jacoline	Jl	370.2	40	94	40	138	30	5.85	senecionine	jacobine
44	jacoline-N-oxide	Jl-ox	386.2	40	94	40	120	30	4.20	senecionine	jacobine-N-oxide
45	jaconine	Jn	388.2	40	94	40	120	30	8.51	senecionine	jacobine
46	jaconine-N-oxide	Jn-ox	404.2	40	94	40	120	35	5.60	senecionine	jacobine-N-oxide
47	jacozine	Jz	350.2	40	94	40	120	30	7.00	senecionine	jacobine
48	jacozine-N-oxide	Jz-ox	366.2	40	94	40	118	30	4.98	senecionine	jacobine-N-oxide
49	lasiocarpine	Las	412.2	30	120	25	220	20	11.10	heliotrine	lasiocarpine
50	lasiocarpine-N-oxide	Las-ox	428.2	30	138	30	254	25	7.92	heliotrine	lasiocarpine-N-oxide
51	lycopsamine	Lyc	300.2	30	94	35	156	30	6.35	lycopsamine	lycopsamine
52	lycopsamine-N-oxide	Lyc-ox	316.2	30	94	40	172	30	4.76	lycopsamine	lycopsamine-N-oxide
53	monocrotaline	Mc	326.2	40	94	35	120	30	6.15	monocrotaline	monocrotaline
54	monocrotaline-N-oxide	Mc-ox	342.2	40	120	35	137	30	4.13	monocrotaline	monocrotaline-N-oxide
55	onetine	On	400.2	30	122	30	168	30	4.25	otonecine	otosene
56	otosene	Ot	382.2	30	168	25	122	30	5.40	otonecine	otosene
57	retorsine	Rt	350.2	40	94	40	120	30	8.26	senecionine	retorsine
58	retorsine-N-oxide	Rt-ox	368.2	40	94	40	120	30	5.80	senecionine	retorsine-N-oxide
59	riddelline	Rd	350.2	40	94	40	120	30	7.67	senecionine	riddelline
60	riddelline-N-oxide	Rd-ox	366.2	40	94	40	118	30	5.25	senecionine	riddelline-N-oxide
61	rinderine	Rin	300.2	30	138	30	156	30	7.10	lycopsamine	lycopsamine
62	rinderine-N-oxide	Rin-ox	316.2	30	111	40	172	30	5.04	lycopsamine	lycopsamine-N-oxide
63	senecionine	Sn	336.2	40	94	40	120	30	9.63	senecionine	senecionine
64	senecionine-N-oxide	Sn-ox	352.2	40	94	40	120	30	6.73	senecionine	senecionine-N-oxide
65	seneciphylline	Sp	334.2	40	120	30	138	30	8.90	senecionine	seneciphylline
66	seneciphylline-N-oxide	Sp-ox	350.2	40	94	40	138	30	6.20	senecionine	seneciphylline-N-oxide
67	senecivermine	Sv	336.2	40	94	40	120	30	9.80	senecionine	integerrimine
68	senecivermine-N-oxide	Sv-ox	352.2	40	94	40	120	30	6.86	senecionine	integerrimine-N-oxide
69	senkirkine	Sk	366.2	30	122	30	168	25	7.12	otonecine	senkirkine
70	spartioidine	St	334.2	40	120	30	138	30	8.75	senecionine	seneciphylline
71	spartioidine-N-oxide	St-ox	350.2	40	94	40	120	30	6.05	senecionine	seneciphylline-N-oxide
72	supinine	Sup	284.2	30	122	20	140	25	8.95	lycopsamine	lycopsamine
73	supinine-N-oxide	Sup-ox	300.2	30	138	30	156	30	5.55	lycopsamine	lycopsamine-N-oxide
74	trichodesmine	Td	354.2	40	120	35	222	30	8.43	monocrotaline	trichodesmine
75	trichodesmine-N-oxide	Td-ox	370.2	40	137	30	238	30	5.80	monocrotaline	trichodesmine-N-oxide
76	usaramine	Us	352.2	40	94	40	120	30	8.10	senecionine	retorsine
77	usaramine-N-oxide	Us-ox	368.2	40	94	40	120	30	5.67	senecionine	retorsine-N-oxide